Methyl salicylate 119-36-8 | DTXSID5025659

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 10.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.39e-01

Confidence level: 5.16e-01

Nearest Neighbors from the Training Set

Image not found

Methyl salicylate Measured: -8.00 Predicted: 10.6 Image not found

Ethyl salicylate Measured: 1.00 Predicted: 17.5 Image not found

Benzoic acid, 2-hydroxy-5methyl-, methyl ester Measured: -1.00 Predicted: 22.6

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Propyl salicylate Measured: 97.0 Predicted: 38.9